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Lattice QCD with a twisted mass term and a strange quark

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Abstract. There are three quarks with masses at or below the characteristic scale of QCD dynamics: up, down and strange. However, twisted mass lattice QCD relies on quark doublets. Various options for including three quark flavors within the twisted mass approach are explored by studying the kaon masses, both analytically (through chiral Lagrangians) and numerically (through lattice simulations). Advantages and disadvantages are revealed for each "strange and twisted" option.

PACS. 11.15.Ha Lattice gauge theory – 12.39.Fe Chiral lagrangians – 14.40.Aq π, K and η mesons

1 Two flavor twisted mass lattice QCD

Consider a hypercubic lattice in four-dimensional space-time, and a two flavor system:

$$\psi(x) = \begin{pmatrix} u(x) \\ d(x) \end{pmatrix} . \tag{1}$$

In the $m_u = m_d \equiv m_q$ limit, the fermion action for twisted mass lattice QCD is

$$S_{\text{fermion}} = a^4 \sum_x \bar{\psi}(x) \left[D(r,\omega) + m_q \right] \psi(x) , \tag{2}$$

with Dirac and Wilson terms,

$$D(r,\omega) = \gamma \cdot \nabla + \exp(-i\omega\gamma_5\tau_3) W(r) , \tag{3}$$

$$W(r)\psi(x) \equiv M_{cr}(r)\psi(x) - \frac{ar}{2} \Box \psi(x) . \tag{4}$$

As usual, the covariant derivative ∇_μ and d'Alembertian $\Box$ contain the gauge field $U_\mu(x) \equiv \exp(iagT^b A^b_\mu(x))$.

Two key features of twisted mass lattice QCD are (a) the existence of a firm lower bound for the eigenvalues of $D(r,\omega) + m_q$, as long as m_q and ω are non-zero[1] and (b) the absence of $O(a)$ errors in observable quantities at maximal twist, $\omega(renormalized) = \pm\pi/2$[2]. Another significant consequence of $\omega \neq 0$ is that parity and flavor symmetries are broken; they only get restored in the continuum limit.

2 Options for including the strange quark

Given the phenomenological importance of u, d, s physics, how should the strange quark be added to the two flavor twisted mass theory of the previous section?

One option is to leave the strange quark untwisted. It will not be protected from near-zero modes, but this is not a practical problem for simulations at the physical strange quark mass. There will be $O(a)$ errors in the theory, but one could remove their effects on observables through addition of a Sheikholeslami-Wohlert term[3]. Kaon operators, containing one twisted and one untwisted fermion, would appear as parity mixtures, requiring extra effort for the extraction of continuum physics.

Another option is to twist the strange quark by using the charm quark as its twisting partner. To accommodate $m_c \neq m_s$, the action for this "heavy" doublet will need one additional term relative to the "light" doublet action used in the previous section for up and down. The quark mass terms in the twisted basis are

$$\begin{aligned} \mathcal{L} &= \bar{\psi}_l \left(m_l + i\gamma_5\mu_l\tau_3 \right) \psi_l \\ &+ \bar{\psi}_h \left(m_h + i\gamma_5\mu_h\tau_3 + \epsilon\tau_a \right) \psi_h , \end{aligned} \tag{5}$$

where τ_a is a Pauli matrix in flavor space. Should we choose $\tau_a = \tau_3$[4] or $\tau_a \neq \tau_3$[5]? An advantage of the parallel choice, i.e. $\tau_a = \tau_3$, is that flavors do not mix, but an important disadvantage is that the fermion determinant is not real. Therefore this parallel choice corresponds to fermions that can be used as valence quarks but not as sea quarks. The perpendicular choice, $\tau_a \neq \tau_3$, leads to a real fermion determinant so those quarks can be both sea and valence, but the flavors in the action mix, as is evident from (5). To elucidate the flavor and isospin structure of this choice, we study the kaon masses in this work.

The notation $(c,s)_\parallel$ and $(c,s)_\perp$ will respectively denote twisted doublets with the parallel and perpendicular choices for τ_a relative to τ_3. A degenerate doublet is denoted by $(u,d)_0$. The three scenarios to be explored are

scenario 1: $(u,d)_0 + s$ [$+c$ if desired] ,
scenario 2: $(u,d)_0 + (c,s)_\parallel$,
scenario 3: $(u,d)_0 + (c,s)_\perp$.

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3 Kaon mass splittings and lattice artifacts

3.1 Chiral perturbation theory

The chiral Lagrangian for two twisted doublets is[6]

$$\mathcal{L}_{\chi PT} = \mathcal{L}^{(2)} + \mathcal{L}^{(4)} + \dots, \tag{6}$$

$$\mathcal{L}^{(2)} = \frac{f^2}{4}\mathrm{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4}\mathrm{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) - \frac{f^2}{4}\mathrm{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}), \tag{7}$$

$$\mathcal{L}^{(4)} = -W_8'\mathrm{Tr}\left[(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A})^2\right] + \dots, \tag{8}$$

where

$$\Sigma = \begin{pmatrix} e^{i\omega_l\tau_3/2} & 0 \\ 0 & e^{i\omega_h\tau_3/2} \end{pmatrix} e^{i\Phi/f} \begin{pmatrix} e^{i\omega_l\tau_3/2} & 0 \\ 0 & e^{i\omega_h\tau_3/2} \end{pmatrix} \tag{9}$$

for meson matrix Φ. The quark mass matrix appears as

$$\chi = 2B \begin{pmatrix} m_l + i\mu_l\tau_3 & 0 \\ 0 & m_h + i\mu_h\tau_3 + \epsilon_h\tau_a \end{pmatrix}, \tag{10}$$

and the lattice spacing as $\hat{A} = 2W_0 a$, using notation familiar from [7,8,9].

To interpret $(u,d)_0 + (c,s)_\perp$, we diagonalize the quark mass matrices,

$$m_l + i\mu_l\tau_3 = \sqrt{m_l^2 + \mu_l^2}\, e^{i\tau_3\omega_l}, \tag{11}$$

$$m_h + i\mu_h\tau_3 + \epsilon_h\tau_1 = e^{i\tau_3\omega_h/2} Y^\dagger M Y e^{i\tau_3\omega_h/2}, \tag{12}$$

where $Y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ is a standard $\pi/4$ rotation, and the diagonal matrix M is

$$M = \begin{pmatrix} \sqrt{m_h^2 + \mu_h^2} + \epsilon_h & 0 \\ 0 & \sqrt{m_h^2 + \mu_h^2} - \epsilon_h \end{pmatrix}. \tag{13}$$

The resulting mass terms for kaons and D mesons have the form

$$(\mathbb{K}^+ \ \bar{\mathbb{D}}^0 \ \mathbb{K}^0 \ \mathbb{D}^-) \begin{pmatrix} m-\delta & \alpha & 0 & 0 \\ \alpha & m+\delta & 0 & 0 \\ 0 & 0 & m-\delta & -\alpha \\ 0 & 0 & -\alpha & m+\delta \end{pmatrix} \begin{pmatrix} \mathbb{K}^- \\ \mathbb{D}^0 \\ \bar{\mathbb{K}}^0 \\ \mathbb{D}^+ \end{pmatrix} \tag{14}$$

where m, δ and α contain various parameters from the chiral Lagrangian. Here, mesons are labelled by their identities in the untwisted limit. They are clearly not mass eigenstates for nonzero twist, $\alpha \neq 0$. To determine meson eigenstates for a general twist, we diagonalize the matrix in (14) through a simple change of basis, and obtain the eigenstates and eigenvalues of Table 1. The rotation (not twist!) angle, $0 \leq \theta < \pi/2$, is given by

$$\tan 2\theta = \left|\frac{\alpha}{\delta}\right|, \tag{15}$$

where $\alpha \sim \sin\omega_l \sin\omega_h$ vanishes if either (u,d) or (c,s) is not twisted, and $\delta \sim \epsilon_h$ vanishes when (c,s) has no explicit mass splitting term.

Table 1. Eigenvalues and eigenstates of the matrix in (14). Note that, for general θ, none of these mass eigenstates are isospin partners.

mass eigenstates	mass eigenvalues
$\psi_{u-} = \mathbb{K}^+\cos\theta - \mathbb{D}^0\sin\theta$	
$\psi_{d-} = \mathbb{K}^0\cos\theta + \mathbb{D}^-\sin\theta$	$m_{u-} = m_{d-} = m - \sqrt{\delta^2+\alpha^2}$
$\psi_{u+} = \mathbb{K}^+\sin\theta + \bar{\mathbb{D}}^0\cos\theta$	
$\psi_{d+} = \mathbb{K}^0\sin\theta - \mathbb{D}^-\cos\theta$	$m_{u+} = m_{d+} = m + \sqrt{\delta^2+\alpha^2}$

Is there a correspondence between these eigenstates and the physical mesons? As a special case, consider $\alpha = 0$. This implies $\theta = 0$ and leads to scenario 1: $(u,d)_0 + s + c$. Quark flavors do not mix; the physical kaons are a (lighter) degenerate isospin doublet, and the physical D mesons are a (heavier) degenerate isospin doublet. This scenario is also discussed in [10].

As a different special case, consider $\delta = 0$. This implies $\theta = \pi/4$ and leads to $(u,d)_0 + (c,s)_0$. Quark flavors can now be diagonalized, and mixings are thus avoided. In fact, this special case then becomes identical to $(u,d)_0 + (c,s)_\parallel$ with $m_c = m_s$. The mass-degenerate doublets are (K^+, D^-) and $(K^0, \bar{D}^0)$. The physical kaons only become degenerate in the continuum limit.

In general, when $\alpha \neq 0$ and $\delta \neq 0$, Table 1 corresponds to $(u,d)_0 + (c,s)_\perp$. The light quark doublet has no flavor mixing, but the heavy doublet does. Interestingly, none of the mass eigenstates form isospin doublets unless isospin is somehow defined to involve (c,s) as well as (u,d). Our findings are sketched in Fig. 1. Scenario 1 has no isospin splittings among kaons, and none among D mesons either, but there are $O(a)$ splittings between the kaons and D mesons. In scenario 2 all splittings begin at $O(a^2)$, but twist artifacts do cause unphysical $O(a^2)$ isospin splittings between charged and neutral kaons, and also between charged and neutral D mesons. In scenario 3, flavors mix. There are two degenerate pairs of eigenstates, but the symmetry relating the degenerate states involves both quark doublets. Identification of these states with physical particles only becomes clear upon extrapolation to the continuum limit.

3.2 Lattice QCD simulations

According to the chiral Lagrangian discussion above, the splitting $m^2(K^0) - m^2(K^\pm)$ that arises from twist artifacts in the $(u,d)_0 + (c,s)_\parallel$ scenario should be, at leading order, (i) independent of quark mass, (ii) linear in a^2, and (iii) vanishing as $a^2 \to 0$. Quenched numerical simulations for this scenario[6,11] are consistent with these expectations, though the vanishing of the mass splitting as $a^2 \to 0$ is not as clear in the data as one might have hoped. Even at the smallest lattice spacing, $a \approx 0.068$ fm, the kaon mass splitting is found to be sizeable: $m(K^0) - m(K^\pm) \sim 50$ MeV.

Ref. [6] also contains quenched results for the $(u,d)_0 + s$ scenario, and these confirm the chiral Lagrangian claim of $m(K^0) = m(K^\pm)$, i.e. the kaon masses are not split by twist artifacts.

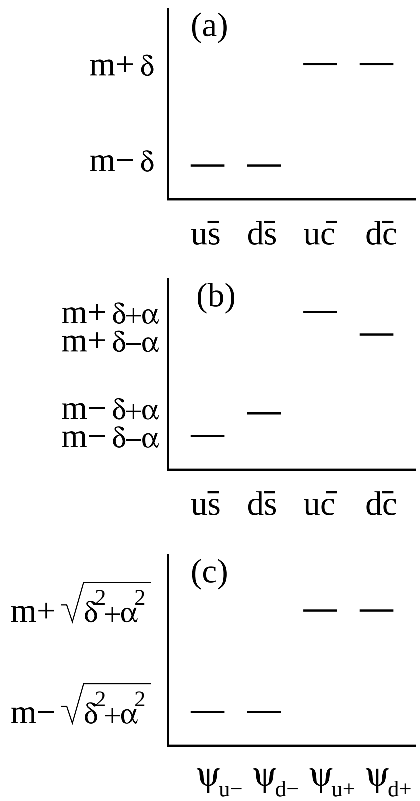

Fig. 1. Meson mass eigenstates obtained from three scenarios, (a) scenario 1: $(u, d)_0 + s + c$, (b) scenario 2: $(u, d)_0 + (c, s)_\parallel$, (c) scenario 3: $(u, d)_0 + (c, s)_\perp$.

For scenario 3, $(u, d)_0 + (c, s)_\perp$, conventional isospin is only restored in the continuum limit. Therefore meson mass eigenstates must be identified by computing the full meson correlation matrix and then diagonalizing it numerically. With quark mass terms

$$\mathcal{L} = (\bar{u}\ \bar{d}) \begin{pmatrix} m_l + i\gamma_5\mu_l & 0 \\ 0 & m_l - i\gamma_5\mu_l \end{pmatrix} \begin{pmatrix} u \\ d \end{pmatrix} + (\bar{q}_1\ \bar{q}_2) \begin{pmatrix} m_h + i\gamma_5\mu_h & \epsilon_h \\ \epsilon_h & m_h - i\gamma_5\mu_h \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \tag{16}$$

and operators $O_{ui} = \bar{u}\gamma_5 q_i$ and $O_{di} = \bar{d}\gamma_5 q_i$, numerical results give

$$C_{ij}^{(u)} \equiv \left\langle O_{ui} O_{uj}^\dagger \right\rangle \Rightarrow C^{(u)} = \begin{pmatrix} a & c \\ c & b \end{pmatrix}, \tag{17}$$

$$C_{ij}^{(d)} \equiv \left\langle O_{di} O_{dj}^\dagger \right\rangle \Rightarrow C^{(d)} = \begin{pmatrix} b & c \\ c & a \end{pmatrix}, \tag{18}$$

where a, b and c are real-valued. Diagonalization of $C^{(u)}$ and $C^{(d)}$ provides the meson mass eigenstates. Simulation results[12,13] are consistent with our chiral Lagrangian discussion.

4 Summary

Twisted mass lattice QCD removes $O(a)$ errors and unphysical near-zero modes. The up and down quarks fit natually into a twisted doublet but the strange quark has no natural partner. Three scenarios for including the strange quark were considered within chiral perturbation theory, and found to have the following features:

- $(u, d)_0 + s + c$
  - no unphysical mass splittings within isospin multiplets,
  - the strange quark does not benefit from twisting,
  - kaon operators (i.e. twisted+untwisted) require care,
- $(u, d)_0 + (c, s)_\parallel$
  - all quarks benefit from twisting,
  - suitable for valence quarks but not for sea quarks,
  - flavors do not mix and isospin is easily managed,
  - discretization effects appear as kaon mass splittings,
- $(u, d)_0 + (c, s)_\perp$
  - all quarks benefit from twisting,
  - dynamical simulations can use a single action,
  - flavors mix; isospin is not straightforward for $a \neq 0$.

These features have also been observed in explicit numerical simulations, and may be helpful when choosing which scenario is optimal for a particular phenomenological application of lattice QCD.

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